ΣΕΜΙΝΑΡΙΟ ΚΕΝΤΡΟΥ ΚΒΑΝΤΙΚΗΣ ΠΟΛΥΠΛΟΚΟΤΗΤΑΣ & ΝΑΝΟΤΕΧΝΟΛΟΓΙΑΣ/ CCQCN SEMINAR

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11:00-12:00

3rd Floor Seminar Room

Structural and dynamical heterogeneities of liquid water near the glass transition

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Abstract

Liquid water features a broad range of dynamics, whose characteristic timescales span from a few femtoseconds at ambient conditions, to seconds near the hypothesized glass transition. The hydrogen bond network is heterogeneous both structurally and dynamically and is responsible for the unusual temperature dependence of the thermodynamic response functions of liquid and supercooled water [1],[2]. It has been suggested that water features two distinct phases with different density (high and low density liquid – HDL and LDL) emerging from the corresponding high and low density amorphous states (HDA and LDA) of water [3]. Can one observe the manifestation of HDL and LDL near the glass transition and is there a first order phase transition between HDL and LDL? Here, we present an overview of our recent experiments investigating the dynamics of liquid water at different timescales. Using X-ray Photon Correlation Spectroscopy[4], we investigate the slower dynamics near the glass transition of LDA and HDA ices and gradually increase the temperature. In this case the small angle scattering geometry enables us to access information about density heterogeneities that extend over several nanometers[5]. The observed dynamics speed up several orders of magnitude as we approach the glass transition, indicating the transition to an ultraviscous liquid state. Complementary, we study the dynamics of liquid water in the picosecond regime, by optical pumping (800nm) and probing with x-ray diffraction. In this case the observed Optical Kerr effect signal reveals information about the timescale of the molecular rearrangement of the liquid water, which are compared to those obtained by 2D-IR spectroscopy[6], [7]. Finally, we investigate the motion in the sub-100fs regime, where motion is dominated by intermolecular vibrations. In a wide-angle scattering geometry, we demonstrate the possibility of resolving the motion associated with neighboring water molecules that occurs within the 50 fs pulse duration.

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